Separation materials: An ace in the hole
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"Porous graphene" makes an excellent separation membrane for hydrogen purification

Original article citation

Several experimental groups have prepared two-dimensional (2D) polyphenylene, a polymer that resembles graphene structurally but has atom-sized pores. Zhen Zhou at Nankai University in Tianjin and co-workers have now used density functional theory calculations to show that 2D polyphenylene exhibits semiconducting characteristics. They also found that the pores endow the structure with the ability to separate hydrogen from other gases.

The researchers computed the band structure and density of states of an optimized 2D polyphenylene structure (see image). They found that 2D polyphenylene has a wide bandgap of 2.48 eV, which is quite different to graphene, which is a semimetal with zero bandgap.

Furthermore, the diffusion energy barrier for H₂ to pass through the pores is much smaller than that for CO₂, CO and CH₄, making 2D polyphenylene 10⁻³³ times more selective for hydrogen compared to traditional silica and carbon separation membranes. The researchers believe that 2D polyphenylene has great potential for hydrogen purification applications.

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Reference